

CONCENTRATION FLUCTUATION DEGRADATION OF FPA'S

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ABSTRACT

Semiconductor alloys like $Hg_{1-x}Cd_xTe$ and $Al_{1-x}Ga_xAs$, where there is a close lattice constant match between the constituents, are nearly random. However, for mesoscopic size scales of radius r , that are large compared with a lattice constant ($\sim 25 \text{ \AA} < r < \sim 250 \text{ \AA}$), but small compared with typical device dimensions, the number of substitutional sites is small enough so the root-mean-square concentration, $(\Delta x)^2^{1/2}$, is sufficiently large to produce random arrays of mesoscopic "quantum dots" that can adversely affect many device properties. The influence of the adverse effects differ among various properties—for example, electron and hole mobilities, lifetimes, and so on—but in general are expected to be worse the smaller the fundamental gap becomes. These kinds of fluctuations are suppressed in lattice-mismatched alloys like $Hg_{1-x}Zn_xTe$ and $Ga_{1-x}In_xAs$ because there is a long-range strain energy penalty associated with them. Thus, lattice-mismatched alloys are more spatially uniform than lattice-matched alloys. In this paper, a calculation of the impact of concentration fluctuations, among regions large enough so it is appropriate to assign them a band structure ($\sim 390 \times 780 \times 780 \text{ \AA}^3$), on tunneling currents is presented. An enhancement of ~ 1.20 ($\sim 20\%$) in the average tunneling current density for LWIR material is found, and its root mean square deviation is ~ 0.90 . For $25 \text{ }\mu\text{m}$ sized pixels this translates to 0.3% variations among pixels due to this effect. This estimate does not include the impact of smaller regions that must be treated quantum mechanically. As pixel sizes decrease the impact of this variation will become more significant. Surprisingly, the effect of fluctuations on the leakage current characteristics of VLWIR ($20 \text{ }\mu\text{m}$ cut off) pixels is also small.

Alloys of the semimetal $HgTe$ with the semiconductor $CdTe$ and with other II-VI semiconductors can have their band gap engineered by varying the proportion of the constituent compounds. For many applications, such as the use of such alloys as detectors in infrared focal plane arrays, it is important that the devices of the array (pixels) be uniform, and that the material within each pixel be homogeneous. Variations in alloy composition within a pixel, and among pixels, can degrade system performance.

The lattice parameters of $ZnTe$ and $CdTe$ are significantly different, unlike $HgTe$ and $CdTe$, which are almost perfectly lattice matched. The energetic consequences of this difference tend to reduce composition fluctuations in the Zn -bearing alloy.

The lattice parameters of most ternary III-V or II-VI semiconductor alloys of composition $A_{1-x}B_xC$ follow Vegard's law quite accurately, with little bowing.¹ When the compounds AC and BC are lattice matched—for example, $Al_{1-x}Ga_xAs$ or $Hg_{1-x}Cd_xTe$ —the cations A and B are randomly distributed

1. Chen, A.-B. and A. Sher, "Semiconductor Alloys," Plenum Press, New York, 1995, 4.

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on the fcc cation sublattice, and deviations of the local composition from the average x are determined purely by statistics. When there is a lattice mismatch, any region of the alloy whose composition deviates from x would have a corresponding unstressed lattice parameter, and therefore must be either compressed or dilated in order to fit into the space available to it. In a paper which linked the mixing enthalpy parameter of such alloys with their bulk elastic properties,^{2,3} it was suggested that the associated elastic energy might reduce composition fluctuations, and the suggestion was quantified for $Al_{1-x}Ga_xAs$ and $In_{1-x}Ga_xAs$. In a later paper, the magnitude and density of concentration fluctuations in $Hg_{1-x}Cd_xTe$ and $Zn_{(1-x)}Cd_xTe$ were presented.⁴

In the absence of any elastic strain, the mean square of a deviation Δx from the average composition x of a region containing N cations ions is

$$\overline{(\Delta x)^2} = \frac{\bar{x}(1-\bar{x})}{N} . \quad (1)$$

The elastic energy density of such a region is^{2,3}

$$W = 18B \left(\frac{a-b}{a+b} \right)^2 (\Delta x)^2 , \quad (2)$$

where a and b are the lattice parameters, and B is the bulk modulus of the alloy.

This energy and the mixing entropy of the alloy were used³ in the thermodynamic formula for the macroscopic composition fluctuations to show that the mean square fluctuations in a lattice-mismatched alloy are reduced below those in a lattice-matched alloy by a factor

$$f = \left(1 + \frac{3WV}{2RT} \bar{x}(1-\bar{x}) \right)^{-1} ; \quad \overline{(\Delta x)^2} = f \frac{\bar{x}(1-\bar{x})}{N} , \quad (3)$$

where V is the molar volume of the alloy, R is the gas constant, and T is the temperature. The appropriate value of T is the growth or annealing temperature at which the alloy reaches equilibrium before cooling.

In the application we are considering here, the primary concern is the occurrence of defects which modify the performance of a pixel. The defects discussed here are not defects in the usual sense, such as impurities or vacancies, but regions in the absorption layer or junction plane whose composition (and therefore whose band gap) differs from the average.

In a random alloy, the distribution of cation populations, $P(x)$, is binomial; the binomial distribution is closely approximated by a Gaussian distribution for as few ions as the 12 ions comprising a single nearest neighbor cation shell.

$$P(x) = \frac{1}{\sqrt{2\pi} (\Delta x)^2} e^{-\frac{(x-\bar{x})^2}{2(\Delta x)^2}} , \quad (4)$$

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2. Fedders, P.A. and M.W. Muller, *J. Phys. Chem. Solids*, 1984, 43, 685; see also Chen, A.-B. and A. Sher, "Semiconductor Alloys," Plenum Press, New York, 1995, 91-92.
 3. Muller, M.W., *Phys. Rev.*, 1984, B30, 6196.
 4. Muller, M.W. and A. Sher, *Appl. Phys. Letters*, 1999, 74, 2343.

where $\Delta x = \bar{x}$.

Figure 1 shows, as deduced in Reference 4, the average distance between defects as a function of Δx_{\min} , the departure of the composition from the average, for defects containing 216, 1,730, 5,830, 13,800, and 27,000 cations, in $Hg_{1-x}Cd_xTe$ with $x = 0.225$ and in $Hg_{1-x}Zn_xTe$ with $x = 0.18$. For regions of $Hg_{0.22}Cd_{0.78}Te$ with a size (diameter) of $\sim 60 \text{ \AA}$ and $\Delta x_{\min} > 1.7\%$, the separation between the mesoscopic regions exceeds their size, so they do not overlap and can be treated as isolated. Smaller regions or lower Δx_{\min} overlap and are meaningless. While the fluctuations of regions with size scales $> 60 \text{ \AA}$ are real, these regions cannot be treated as though they have a distinct band gap unless their size exceeds a de Broglie wavelength λ_{dB} .

$$\lambda_{dB} \cong \frac{h}{\sqrt{2m^* E_g}} \quad . \quad (5)$$

The energy we have used to specify λ_{dB} is the band gap E_g . For regions smaller than λ_{dB} a full quantum mechanical treatment is required. Let us concentrate for now on size scales larger than λ_{dB} .

The immediate concern is on tunneling leakage currents. Other properties relevant to device performance are impacted by fluctuations but will not be treated here. The tunneling rate, $T(x)$ across a reverse biased junction is:⁵

$$T(x) \propto \exp \left[\frac{\pi}{2\sqrt{2}} \frac{m^{*1/2}}{eE\hbar} E_g^{3/2} \right] \quad (6)$$

where m^* is the electron effective mass, e is the electron charge, and the relevant field (E) is the band gap divided by the depletion layer thickness L ,

$$E = E_g / L \quad . \quad (7)$$

If the junction interface is divided into regions that are one a de Broglie wavelength thick and $(2\lambda_{dB})^2$ in cross sectional area, then the average tunneling rate across these regions is,

$$\langle T \rangle \propto \int_a^u dx P(x) T(x) \quad , \quad (8)$$

where, for lattice constant a ,

$$N = 16 \left(\frac{\lambda_{dB}}{a} \right)^3 \quad . \quad (9)$$

5. Sze, S.M., "Physics of Semiconductor Devices," Second Edition, John Wiley, New York, 1981.

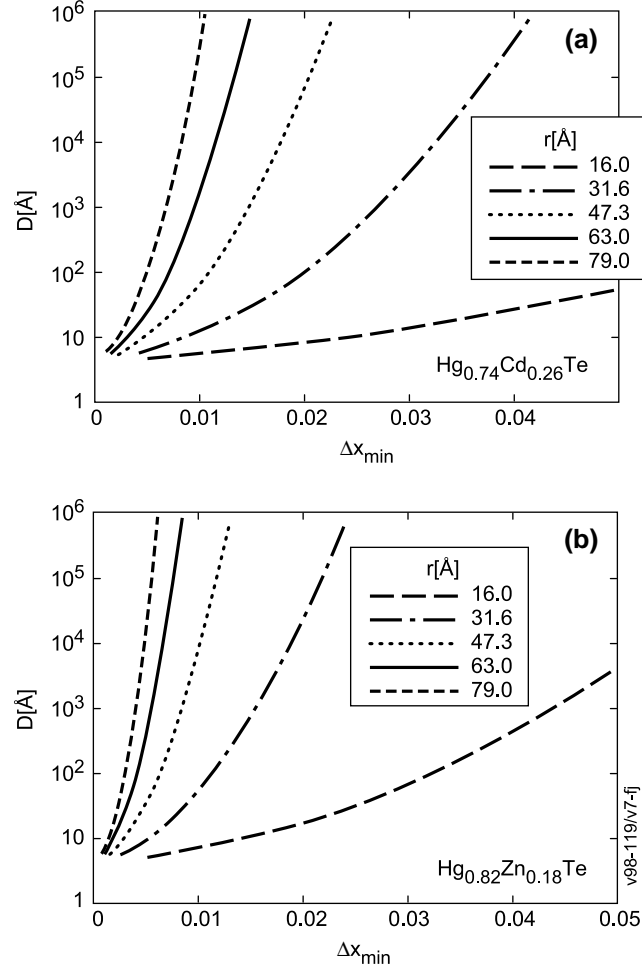


Figure 1. Concentration Fluctuations, $\lambda_c = 10 \mu\text{m}$.

- (a) $\text{Hg}_{1-x}\text{Cd}_x\text{Te}$, $x = 0.26$. The average separation $D[\text{\AA}]$ between spherical regions of radius $r[\text{\AA}]$ with magnitudes greater than a specified minimum x_{\min} , plotted against x_{\min} .
- (b) $\text{Hg}_{1-x}\text{Zn}_x\text{Te}$, $x = 0.18$, equilibrated at $T = 220^\circ \text{C}$. The average separation $D[\text{\AA}]$ between spherical regions of radius $r[\text{\AA}]$ with magnitudes greater than a specified minimum x_{\min} , plotted against x_{\min} .

The factor of 16 arises because there are 4 cations per unit cell and the volume of the mesoscopic regions being used is $4(\lambda_{\text{dB}})^3$. The gap energy as a function of x can be approximated by

$$E_g(x) \cong E_g(\bar{x}) + \frac{dE_g(\bar{x})}{dx} \Delta x \quad (10)$$

and

$$E_g^{3/2}(x) \cong E_g^{3/2}(\bar{x}) + \frac{3}{2} \frac{dE_g(\bar{x})}{dx} E_g^{1/2}(\bar{x}) \Delta x \quad (11)$$

Inserting Eq. (8) into Eq. (11) and integrating yields,

$$\frac{\langle T \rangle}{T(\bar{x})} = e^\alpha \quad , \quad (12)$$

where α is defined as,

$$\begin{aligned} \alpha &\equiv \frac{1}{2} \left[\frac{\bar{x}(1-\bar{x})}{N} \left[\frac{\pi}{2\sqrt{2}} \frac{m^{*1/2}}{eE\hbar} E_g^{3/2}(\bar{x}) \right]^2 \left[\frac{3}{2} \frac{dE_g(\bar{x})}{dx} E_g^{1/2}(\bar{x}) \right]^2 \right. \\ &\quad \left. \equiv 1.0 \times 10^{-3} \frac{E_g^{1/2} \left(\frac{dE_g}{dx} \right)^2 m^{*5/2} a^3 L^2 \bar{x}(1-\bar{x})}{\hbar^5} \right] \end{aligned} \quad (13)$$

The root mean square tunneling rate can also be found in closed form, and is,

$$\frac{\langle (\Delta T)^2 \rangle^{1/2}}{T(\bar{x})} = e^\alpha (e^{2\alpha} - 1)^{1/2} \quad . \quad (14)$$

Finally the current I , through a pixel of size w , is the sum of the currents through the array of mesoscopic regions within the pixel, so we have, $\langle I / I(\bar{x}) \rangle = \langle T / T(\bar{x}) \rangle$. The deviations in the currents through each mesoscopic region add in quadrature so $\langle (\Delta I)^2 \rangle = (\text{the number of mesoscopic regions per pixel})^{-1/2} \langle (\Delta T)^2 \rangle$, which is,

$$\frac{\langle (\Delta I)^2 \rangle^{1/2}}{I(\bar{x})} = \frac{1}{(w / 2\lambda_{dB})} \frac{\langle (\Delta T)^2 \rangle^{1/2}}{T(\bar{x})} \quad . \quad (15)$$

As long as $w \gg \lambda_{dB}$ ($\approx 390 \text{ \AA}$ for 10 \mu m cutoff material), the variation in the leakage currents from pixel to pixel will be modest.

DISCUSSION

The results for various quantities are collected in Table 1. Aside from the numbers reported in Table 1, the quoted results depend on the following parameters, $dE_g/dx = 1.7[\text{eV}]$, $L = 1[\text{\mu m}]$, and $a = 6.5 \text{ \AA}$.⁶ If the carrier concentration or the operating temperature causes L to change then the results will change appreciably since α is proportional to L^2 , and α enters in an exponential. For the numbers used, the effect of concentration fluctuations on the average leakage current for $\lambda_{co} = 10 \text{ \mu m}$ is only a 20% increase. Surprisingly, the increase in the leakage current for $\lambda_{co} = 20 \text{ \mu m}$ is smaller, 7%. This occurs because the de Broglie wavelength for the 20 \mu m cutoff material is larger causing the size of the mesoscopic regions considered to be larger. The smaller sized regions still contribute to the leakage current even though this analysis cannot properly treat their influence. To estimate their effects the size of the regions was decreased by a factor η in the analysis. We expect that this over estimates the impact of these smaller regions, since quantum effects are expected to smooth the band structures of these regions.

6. Chen, A.-B. and A. Sher, "Semiconductor Alloys," Plenum Press, New York, 1995.

The size reduction results are collected in Table 2. Notice that as η decreases, $\langle(\Delta I)^2\rangle^{1/2}$ first decreases, and then begins to increase. The initial decrease occurs because $(w/2\lambda_{dB})$ in the denominator of Eq. (15) increases faster than $\langle(\Delta T)^2\rangle^{1/2}$. For smaller η , this situation reverses, and $\langle(\Delta I)^2\rangle^{1/2}$ increases, although it never gets very big.

Table 1. Quantities that Enter the Fluctuation Calculations for Two Cutoff Wavelengths

$\lambda_{co}(\mu m)$	x	$E_g[meV]$	m^*	$\lambda_{dB}[\text{\AA}]$	$N[10^6]$	$E[V/cm]$	$\frac{\langle T \rangle}{T(\bar{x})}$	$\frac{\langle \Delta T^2 \rangle^{1/2}}{T(\bar{x})}$	$\frac{\langle (\Delta I)^2 \rangle^{1/2}}{I(\bar{x})}$
10	0.22	0.12	0.008	390	35	1200	1.20	0.90	0.0056
20	0.19	0.62	0.006	630	15	620	1.07	0.41	0.0032

Table 2. Effect on $\langle(\Delta I)^2\rangle^{1/2} / I(\bar{x})$ of Decreasing the Size of the Mesoscopic Regions by a Factor η

η	$\langle(\Delta I)^2\rangle^{1/2} / I(\bar{x})[\%]$	
	$\lambda_{co} = 10 \mu m$	$20 \mu m$
1	0.56	0.32
1/2	0.45	0.25
1/5	1.50	0.41
1/10	12.00	0.78
1/20	---	2.80

Fluctuations also have consequences on the bulk properties of these alloys. For example, the $r = 31.6 \text{ \AA}$ regions with $\Delta x_{min} = 1.7\langle(\Delta x)^2\rangle^{1/2}$ constitute a random array of “quantum dots” in the conduction band of *HgCdTe* $10 \mu m$ cutoff material with amplitudes of $\pm 20 \text{ meV}$ and average separations of $\sim 70 \text{ \AA}$. The $\Delta x_{min} = 1.7\langle(\Delta x)^2\rangle^{1/2}$ value was chosen as an example because the average separation between such regions is larger than the size of the region, so there is no issue about overlapping regions. For a carrier concentration of $\sim 5 \times 10^{14} \text{ cm}^{-3}$ in such a rough potential arrangement at 0° K (assuming the donor states resonate in the conduction band so there is no carrier freeze out), states up to $\sim 30 \text{ meV}$ will be filled. This estimate assumes that half the volume are valleys, the electrons fill only the valley states, and takes some account of the nonparabolic nature of the conduction band structure. At 77° K the electrons will be spread over an additional $\sim 7 \text{ meV}$. To propagate in this mountain range, electrons must either partially tunnel through or percolate around the hills, or at very low temperature experience “Anderson localization” and “Mott variable range hopping.”⁷ In any case, their mobility will be smaller

7. Mott, N.F. and E.A. Davis, *Electronic Processes in Non-Crystalline Materials*, Clarendon Press,

than if they experience normal drift transport. This behavior in low n-type *HgCdTe* is well documented,⁸ but has never been ascribed to concentration fluctuations. From Figure 1(b) it can be seen that the average separation between fluctuations in *HgZnTe* of magnitude 1.7 % is ~1500 Å rather than the ~70 Å for *HgCdTe* with the same band gap. If the *HgZnTe* is equilibrated at 100° C rather than 220° C, then the separation increases still further to ~1 µm.

When material has a mobility edge, where states above a critical energy have a high mobility and those below this energy have a low mobility, it leads to 1/f noise.^{6,9} Thus, the concentration fluctuations are also a likely source of some of the observed, but unexplained 1/f noise found in systems made from these materials.¹⁰

The fluctuations will impact many other properties important to device applications. The list includes hole mobilities, Shockley-Read-Hall lifetimes (through capture cross sections and ladder states in the gap), and Auger lifetimes (estimated reductions of factors of 3 at higher temperatures to 10 at lower temperatures have been made).¹¹

While *HgZnTe* alloys have been grown by liquid phase epitaxy¹² and molecular beam epitaxy¹³ methods, and some properties characterized, no measurements have been made that have a direct bearing on the predictions of this paper.

Fluctuations can degrade the properties of lattice-matched alloys more than those of lattice-mismatched alloys where they are suppressed. The magnitudes of the effects on various properties must still be computed, but it is clear from the qualitative arguments made here that they will be detrimental. Their suppression in *HgZnTe* should be beneficial to focal plane array performance particularly in the very long wave infrared range.

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